Random error estimation in refractive index measured with the terahertz time domain spectroscopy

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Abstract: This study proposes a practical method to estimate the random error in real part of refractive index measured with terahertz time domain spectroscopy (THz-TDS) for the single measurement of sample by using the phase spectra of the reference terahertz electric field and their standard deviation. The validity of this method is based on the experimental result that the phase correlates with its standard deviation and the signal to noise ratio is almost equal in the phase spectra of reference and sample signal. The random error estimated from the proposed method fitted well to the statistically computed standard deviation.

Keywords: THz-TDS, optical constants, refractive index, random errors

Classification: Science and engineering for electronics

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1 Introduction

Terahertz time domain spectroscopy (THz-TDS) has been rapidly growing as an important technology to obtain the spectroscopic data of wide variety of materials in the terahertz frequency region [1]. The spectroscopic data measured using THz time domain spectrometer is generally affected by various sources of random and systematic errors [2]. However, the report of these errors in optical constants still remains scarce in existing literature and database [3, 4], which is primarily due to the need of large number of data for deriving the standard deviation using statistical mathematics. As the data acquisition of a single THz waveform takes few minutes, taking numbers of data requires several hours, which is not always practical in terms of measurement time and computational efficiency.

Previously, the study on dynamic range to identify the detection limit of the absorption coefficient has been reported by using the intensity spectra of single pair of reference and sample signal measured with the transmission THz-TDS [5]. Also, the study on signal to noise ratio (SNR) in intensity spectra has been reported by taking a large number of measurements [6]. The former study can not discuss the standard deviation in optical constants whereas the latter requires large number of data to analyze the standard deviation in the intensity spectrum. Moreover, these studies are not able to demonstrate the standard deviation in phase spectra. The estimation of random errors in the optical constants like real part of refractive index has to be discussed using the standard deviation in the phase spectra measured with the transmission THz-TDS. Recently, we have proposed a practical method to estimate the standard deviation in the optical constants like transmittance and absorption coefficients, which are derived from the intensity spectra [7]. In this letter, we propose a simple method to estimate the random error in the phase and real part of refractive index by using a single measurement of sample under investigation.

2 Measurement and derivation of standard deviation in phase spectra

We have measured two ZnTe crystals with different thickness of 0.767 mm and 1.496 mm supplied commercially by Nippon Mining and Metals Co. Ltd [8] by using a THz-TDS made by Tochigi Nikon Corp. (Rayfact Spectra) [9] in

transmission geometry. This system uses LT-GaAs photoconductive antennas as THz emitter and detector and a compact femto-second (fs) fiber laser (Femtolute, IMRA Inc.) with a pulse width of less than 100 fs and 20 mW average power as a light source for pumping the emitter and probing the detector. Pulse waveforms of THz electric field are recorded as a sample signal when propagating through the sample under investigation and as a reference signal without a sample. Each time domain signal consists of 1024 data points and measured up to the time delay of 41 ps corresponding to a frequency resolution of 24 GHz.

In our measurement, 12 and 16 pairs of reference and sample data have been recorded for 0.767 mm and 1.496 mm ZnTe samples respectively in a manner like $R_1, S_1, S_2, R_2, \dots, R_k, S_k, \dots, S_{m-1}, S_m, R_m$, where R and S are the reference and sample data respectively, and k and m of subscripts are integers. This type of measurement pattern allows us to make the pair of reference and sample signal taken close to each other in time. From each pair of reference and sample signal like R_k and S_k , transmittance and optical constants like complex refractive index is calculated through the Fourier transforms. Using the simple statistical mathematics, the mean and standard deviation (σ) of these spectra are computed, which is called as σ from statistical mathematics in this literature. This is a regular method to determine the standard deviation.

Pulse waveforms of THz-electric field in time domain are converted through the Fourier transform to the complex spectra in frequency domain. The spectra of electric field are $E_R(\omega) = |E_R(\omega)| \exp\{i\phi_R(\omega)\}$ and $E_S(\omega) = |E_S(\omega)| \exp\{i\phi_S(\omega)\}$ for reference and sample respectively, where $|E(\omega)|$ and $\phi(\omega)$ are spectra of amplitude and phase respectively and ω is the angular frequency. Phase unwrapping, extrapolation from good signal to noise ratio (SNR) region (0.3–0.6 THz) to lower frequencies (< 0.3 THz) and setting zero radian at zero frequency are executed in the derivation of the phase spectra. Transmittance and phase difference are calculated by $T(\omega) = |E_S(\omega)|^2 / |E_R(\omega)|^2$ and $\Delta\phi(\omega) = \phi_S(\omega) - \phi_R(\omega)$ respectively. The averaged phase difference $\langle\Delta\phi\rangle$ and its standard deviation are statistically calculated from the pairs of reference and sample spectra, which are displayed for the 0.767 mm-thick ZnTe sample by dotted lines in Fig. 1.

3 Modeling of standard deviation in phase spectrum

Time domain pulses suffered from the random errors are typically characterized by the irregularities in the amplitude and temporal positions of the pulse peak. The change in the fs laser light and other sources of random errors like electronic circuits, instability of optical and mechanical components used in spectrometer are the responsible factor to produce the variation in the amplitude and position of pulse peaks in time domain measurement. The variation in amplitude of the THz waveform is related to the error in transmittance whereas the shift in temporal position contributes the error in phase. Owning to the latter variations, the THz pulse waveforms, which take about ten

Fig. 1. (a) Phase spectra of reference and 0.767 mm ZnTe sample, and phase differences computed by two methods; one is derived from the averaged reference and sample and another is calculated by statistical mathematics. (b) Standard deviation spectra of reference and sample and phase difference computed by error propagation and also by statistical mathematics.

minutes for single measurement, showed the drift with the measurement time of the order of 100 minutes as well as the smaller random fluctuations. The drifts in pulse peak position existed in both of the reference and sample signals and had a good correlation in terms of measurement time. These drifts are not the random noise and hence they can be removed in the data analysis.

We fitted the variation in pulse peak positions of THz waveform by a second order polynomial to trace the drift and also calculated the average of pulse peak positions. The difference between the fitted curve and the average position was calculated and denoted as δt_i , where i varies from 1 to number of reference or sample data, representing the drift in pulse peak position of THz waveform. The drift can be compensated using δt_i in the phase of Fourier transformed spectra of the THz time domain waveform by the following equation.

$$\phi_i(\omega) = \phi_m(\omega) - \delta t_i \omega, \quad (1)$$

where $\phi_i(\omega)$ and $\phi_m(\omega)$ are the compensated phase and the phase obtained from the measured THz waveform through the Fourier transform respectively. This compensation has been performed for both reference and sample signals and then the mean and standard deviation in the phase of reference ($\langle \phi_R \rangle$ and $\sigma_{\phi,R}$) and sample ($\langle \phi_S \rangle$ and $\sigma_{\phi,S}$) are calculated statistically, which are shown in Fig. 1 (a) and 1 (b) respectively. The phase difference is calculated by subtracting the phase of reference from the sample and the standard deviation in phase difference is determined by using the law of error propa-

gation [10] as

$$\sigma_{\Delta\phi} = (\sigma_{\phi,R}^2 + \sigma_{\phi,S}^2)^{1/2} \quad (2)$$

The phase difference and its standard deviation computed using this method is compared with that calculated directly by statistical mathematics using each pair of reference and sample data in Figs. 1 (a) and 1 (b). This figure shows the two methods are consistent with each other in the phase difference and its standard deviation, meaning that the compensation of drift in the pulse peak position is equivalent to adopting pairs of reference and sample taken close in time for calculating the phase difference.

4 Standard deviation in real part of refractive index

The real part of refractive index $n(\omega)$ is derived from the spectra of transmittance and phase difference by iterative calculation. The following relation between the real part of refractive index and the phase difference is applied in the calculation.

$$n(\omega) = \frac{c}{d\omega} \left[\Delta\phi(\omega) + \frac{d\omega}{c} - \arg(t_{as} \cdot t_{sa}) \right], \quad (3)$$

where c is the velocity of light, d is the sample thickness and t_{as} and t_{sa} are the Fresnel's transmission coefficients of electric field from air to sample and sample to air respectively. By considering the Fig. 1 (a) and 1 (b), we can assume a simple relation between the phase $\phi(\omega)$ and its standard deviation $\sigma_{\phi}(\omega)$ expressed as

$$\sigma_{\phi}(\omega) = C_{\phi} \cdot \phi(\omega), \quad (4)$$

where C_{ϕ} is assumed as a constant which depends on characteristics of the spectrometer as well as the measurement date and condition. We calculated the values of C_{ϕ} from the phase spectra and the standard deviations of sample

Fig. 2. Values of C_{ϕ} for reference and 0.767 mm ZnTe sample. Inset displays the intensity spectra of the reference and sample and the maximum frequency for the detectable signal in the sample spectrum (vertical dashed line).

and reference to verify the validity of Eq. (4). Figure 2 displays the resultant values of C_ϕ , proving that it is almost constant and identical for sample and reference at the frequency region where the signal does not vanish as shown in the inset. We can say that the constant C_ϕ is common in the sample and reference and is practically determined by averaging the values of C_ϕ below the detectable frequency limit.

From the above equation, knowing the value of C_ϕ for a sequence of reference phase spectra enables us to estimate the standard deviation of the sample phase spectra even if it is taken only one time. In the practical application, a number of different samples are measured in a pattern like $R_0, S_0, S_1, R_1, R_2, S_2, \dots, R_k, S_k, \dots, S_{m-1}, S_m, R_m$, where the reference data is taken alternately under the same condition and can be further used to determine the value of C_ϕ . The standard deviation in real part of refractive index $\sigma_{n(\omega)}$ can be computed from the standard deviation in the phase difference $\sigma_{\Delta\phi(\omega)}$ by using the law of error propagation

$$\sigma_{n(\omega)} = \left(\frac{c}{d\omega} \right) \sigma_{\Delta\phi(\omega)}, \quad (5)$$

because the main contributing factor in $\sigma_{n(\omega)}$ is originated from the standard deviation in the phase difference.

Figures 3(a) and 3(b) display the real part of refractive indices and their standard deviations for the 0.767 mm and 1.496 mm ZnTe samples respectively. The estimated standard deviation in Fig. 3(b) was derived by the proposed method of Eq. (4) and the error propagation of Eq. (5). In these cases the value of C_ϕ was adopted as 0.00019 and 0.00036 for 0.767 mm and 1.496 mm-thick ZnTe samples respectively. The standard deviation is also di-

Fig. 3. (a) Mean of refractive indices of 0.767 mm and 1.496 mm ZnTe samples computed by statistical mathematics. (b) Estimated and statistical standard deviations in refractive indices of the ZnTe samples.

rectly calculated by the statistical method using numbers of refractive indices obtained from the pairs of reference-and-sample data and also displayed in Fig. 3(b). Results show that the estimated standard deviation in real part of refractive index is consistent with the standard deviation computed using statistical mathematics up to the detectable frequency limit, indicating the proposed method is appropriate and effective for estimating the standard deviation in the phase and the real part of refractive index. Moreover, it can be seen that the random error in 1.496 mm ZnTe sample is larger than 0.767 mm ZnTe sample and this is primarily because the thicker sample causes larger phase shift.

5 Summary

This study proposes a simple and computationally efficient method to estimate the random error in phase and real part of refractive index measured with transmission THz-TDS. This model is principally based on that the standard deviation in phase is proportional to the phase spectrum itself and the signal to noise ratio is almost equal in the phase spectra of reference and sample signal. Having the knowledge of standard deviation in phase spectra of the reference allows us to estimate the standard deviation in the sample spectra even if the sample is measured only one time. Finally, this study makes it possible to estimate the random errors by implementing the law of error propagation in the real part of refractive index using a limited number of measurements of sample under investigation.

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